Application of the SAFT-Γ Mie Group Contribution Approach to the Modelling of Solubility of Organic Compounds in Solvents and Solvent Mixtures

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The reliable design of novel processes and products postulates the need for accurate thermodynamic tools that are able to describe the thermophysical properties of fluids and fluid mixtures over a wide range of conditions. Versatile equations of state (EoSs) have been developed for this purpose within the general framework of the Statistical Associating Fluid Theory (SAFT) [1,2] that allow for an accurate description of highly non-ideal systems. However, the application of such approaches requires an extensive amount of experimental data available for the accurate characterisation of the substance(s) of interest. This has led to several extensions and re-formulations of SAFT-type theories within the general scope of group contribution approaches [3-6], in an attempt towards more predictive thermodynamic models. A recent example of this family of approaches is the SAFT-γ Mie group contribution theory, a formulation of the SAFT-VR Mie EoS [7,8] within a group contribution formalism, where molecules are modelled as consisting of distinct functional groups that interact via the Mie potential of variable attractive and repulsive range. In this work, we present the application of the SAFT-γ Mie EoS to the study of solubility of organic compounds in solvents and solvent mixtures. The motivation lies in the importance of the prediction of solubility in (mainly) the pharmaceutical and agrochemical industries. Solubility prediction is a very attractive field for the application of predictive thermodynamic models, since in most cases the amount of experimental data for the substance(s) of interest are rather scarce and costly to produce. The advantage of the application of the SAFT-γ Mie EoS in this case lies in the fact that the compounds of interest can be successfully characterised in a group contribution fashion. Complex molecules can be approached based on group parameters for functional groups that have been characterised previously, for which experimental data are generally available (e.g. alkanes, alkanols and aromatic hydrocarbons and, in some cases, mixtures of these). Furthermore, the unusual feature of the SAFT-γ Mie EoS to obtain information of the nature of the unlike interactions between groups from experimental data for pure compounds reduces even more the amount of the necessary experimental data. We will present the group parameters required for the prediction of the solubility of a set of organic compounds and active pharmaceutical ingredients in solvents and solvent mixtures and discuss the quality in the description of the solubility as a function of temperature and composition (for solvent blends).

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